CHAPTER 9

Ordinary Differential Equations

Equations, wherein the unknown quantity is a function rather than a variable and involves derivatives of the unknown function, are known as differential equations. An *ordinary* differential equation is a special case where the unknown function has only one independent variable with respect to which derivatives occur in the equation. If, on the other hand, derivatives of more than one variable occur in the equation, then it is known as a *partial* differential equation, and that is the topic of Chapter 11. This chapter focuses on ordinary differential equations (ODEs) and explores symbolic and numerical methods for solving this type of equation. Analytical closed-form solutions to ODEs often do not exist. But for certain special kinds of ODEs, there are analytical solutions, and in those cases, there is a chance that we can find solutions using symbolic methods. If that fails, we must, as usual, resort to numerical techniques.

Ordinary differential equations are ubiquitous in science and engineering, as well as in many other fields, and they arise, for example, in studies of dynamical systems. A typical example of an ODE is an equation that describes the time evolution of a process where the rate of change (the derivative) can be related to other properties of the process. To learn how the process evolves in time, given some initial state, we must solve or integrate the ODE that describes the process. Examples of applications of ODEs are the laws of mechanical motion in physics, molecular reactions in chemistry and biology, and population modeling in ecology, to mention a few.

This chapter explores both symbolic and numerical approaches to solving ODE problems. The SymPy module is used for symbolic methods; the numerical integration of ODEs uses functions from the integrate module in SciPy.

Importing Modules

Here, the NumPy and Matplotlib libraries are required for basic numerical and plotting purposes, and for solving ODEs, we need the SymPy library and SciPy's integrate module. As usual, let's assume that these modules are imported in the following manner.

```
In [1]: import numpy as np
In [2]: import matplotlib.pyplot as plt
In [3]: from scipy import integrate
In [4]: import sympy
```

For nicely displayed output from SymPy, we need to initialize its printing system.

```
In [5]: sympy.init printing()
```

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Ordinary Differential Equations

The simplest form of an ordinary differential equation is $\frac{dy(x)}{dx} = f(x,y(x))$, where y(x) is the unknown

function and f(x,y(x)) is known. It is a differential equation because the derivative of the unknown y(x) function occurs. Only the first derivative occurs in the equation, which is an example of a first-order

ODE. More generally, we can write an ODE of nth order in explicit form as $\frac{d^n y}{dx^n} = f\left(x, y, \frac{dy}{dx}, \dots, \frac{d^{n-1}y}{dx^{n-1}}\right)$ or in implicit form as $F\left(x, y, \frac{dy}{dx}, \dots, \frac{d^n y}{dx^n}\right) = 0$, where f and F are known functions.

An example of a first-order ODE is Newton's law of cooling $\frac{dT(t)}{dt} = -k(T(t)-T_a)$, which describes

the temperature T(t) of a body in a surrounding with temperature Ta. The solution to this ODE is $T(t) = T_0 + (T_0 - Ta)e^{-kt}$, where T_0 is the initial temperature of the body. An example of a second-order ODE is

Newton's second law of motion F = ma, or more explicitly $F(x(t)) = m \frac{d^2x(t)}{dt^2}$. This equation describes the

position x(t) of an object with mass m when subjected to a position-dependent force F(x(t)). To completely specify a solution to this ODE, we would, in addition to finding its general solution, also have to give the initial position and velocity of the object. Similarly, the general solution of an nth order ODE has n free parameters that we need to specify, for example, as initial conditions for the unknown function and n-1 of its derivatives.

An ODE can always be rewritten as a system of first-order ODEs. Specifically, the *n*th order ODE on the explicit form $\frac{d^n y}{dx^n} = g\left(x, y, \frac{dy}{dx}, \dots, \frac{d^{n-1}y}{dx^{n-1}}\right)$ can be written in the *standard form* by introducing *n* new functions

 $y_1 = y$, $y_2 = \frac{dy}{dx}$, ..., $y_n = \frac{d^{n-1}y}{dx^{n-1}}$. This gives the following system of first-order ODEs:

$$\frac{d}{dx}\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-1} \\ y_n \end{bmatrix} = \begin{bmatrix} y_2 \\ y_3 \\ \vdots \\ y_n \\ g(x,y_1,\ldots,y_n) \end{bmatrix},$$

which also can be written in a more compact vector form: $\frac{d}{dx}\mathbf{y}(x) = f(x,\mathbf{y}(x))$. This canonical form is particularly useful for numerical solutions of ODEs, and it is common that numerical methods for solving ODEs take the $f = (f_1, f_2, ..., f_n)$ function, which in the current case is $f = (y_2, y_3, ..., g)$, as the input that specifies $\frac{d^2 y}{dx^2}$

the ODE. For example, the second-order ODE for Newton's second law of motion, $F(x) = m\frac{d^2x}{dt^2}$, can be

written in the standard form using $\mathbf{y} = \left[y_1 = x, y_2 = \frac{dx}{dt} \right]^T$ giving $\frac{d}{dt} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} y_2 \\ F(y_1)/m \end{bmatrix}$.

If the $f_1, f_2, ..., f_n$ functions are all linear, then the corresponding system of ODEs can be written on the

simple form $\frac{d\mathbf{y}(\mathbf{x})}{dx} = A(x)\mathbf{y}(x) + \mathbf{r}(x)$, where A(x) is an $n \times n$ matrix and $\mathbf{r}(x)$ is an n-vector that only

depends on x. In this form $\frac{dT(t)}{dt} = -k(T(t)-T_a)$, the r(x) is known as the *source term*, and the linear

system is known as *homogeneous* if $\mathbf{r}(x) = 0$ and *nonhomogeneous* otherwise. Linear ODEs are an important special case that can be solved, for example, using eigenvalue decomposition of A(x). Likewise, for certain properties and forms of the $f(x, \mathbf{y}(x))$ function, there may be known solutions and special methods for solving the corresponding ODE problem. But there is no general method for an arbitrary $f(x, \mathbf{y}(x))$, other than approximate numerical methods.

In addition to the properties of the f(x, y(x)) function, the boundary conditions for an ODE also influence the solvability of the ODE problem, as well as which numerical approaches are available. Boundary conditions are needed to determine the values of the integration constants that appear in a solution. There are two main types of boundary conditions for ODE problems: *initial value conditions* and *boundary value conditions*. For initial value problems, the value of the function and its derivatives are given at a starting point, and the problem is to evolve the function forward in the independent variable (e.g., representing time or position) from this starting point. For boundary value problems, the value of the unknown function, or its derivatives, is given at fixed points. These fixed points are frequently the endpoints of the domain of interest. This chapter mostly focuses on initial value problem, and methods that apply to boundary value problems are discussed in Chapter 10 on partial differential equations.

Symbolic Solution to ODEs

SymPy provides a generic ODE solver sympy.dsolve, which can find analytical solutions to many elementary ODEs. The sympy.dsolve function attempts to automatically classify a given ODE, and it may attempt a variety of techniques to find its solution. It is also possible to give hints to the dsolve function, which can guide it to the most appropriate solution method. While dsolve can be used to solve many simple ODEs symbolically, as presented in the following, it is worth keeping in mind that most ODEs cannot be solved analytically. Typical examples of ODEs where one can hope to find a symbolic solution are ODEs of first or second order or linear systems of first-order ODEs with only a few unknown functions. It also helps greatly if the ODE has special symmetries or properties, such as being separable, having constant coefficients, or is in a special form for which known analytical solutions exist. While these types of ODEs are exceptions and special cases, there are many important applications of such ODEs. For these cases, SymPy's dsolve can be a very useful complement to traditional analytical methods. This section explores using SymPy and its dsolve function to solve simple but commonly occurring ODEs.

To illustrate the method for solving ODEs with SymPy, let's begin with a simple problem and gradually look at more complicated situations. The first example is the simple first-order ODE for Newton's cooling law, $\frac{dT(t)}{dt} = -k(T(t)-T_a)$, with the initial value $T(0) = T_0$. To approach this problem using SymPy, we first

need to define symbols for the variables t, k, $T_{_0}$, and $T_{_{a'}}$ and to represent the unknown function T(t), we can use a sympy. Function object.

Next, we can define the ODE very naturally by simply creating a SymPy expression for the left-hand side of the ODE when written on the form $\frac{dT(t)}{dt} + k(T(t) - T_a) = 0$. Here, to represent the T(t) function, we can

now use the SymPy function object T. Applying the symbol t to it, using the function call syntax T(t), results in an applied function object that we can take derivatives of using either sympy.diff or the diff method on the T(t) expression.

In [8]: ode = T(t).diff(t) + k*(T(t) - Ta)
In [9]: sympy.Eq(ode)
Out[9]:
$$k(-T_a+T(t))+\frac{dT(t)}{dt}=0$$

Here sympy.Eq is used to display the equation, including the equality sign and a right-hand side that is zero. Given this representation of the ODE, we can directly pass it to sympy.dsolve, which attempts to automatically find the general solution of the ODE.

```
In [10]: ode_sol = sympy.dsolve(ode)
In [11]: ode_sol
Out[11]: T(t) = C_1e^{-kt} + T_a
```

For this ODE problem, the sympy.dsolve function indeed finds the general solution, which includes an unknown integration constant C_1 that we have to determine from the initial conditions of the problem. The return value from the sympy.dsolve is an instance of sympy.Eq, which is a symbolic representation of equality. It has the lhs and rhs attributes for accessing the left-hand side and the right-hand side of the equality object.

```
In [12]: ode_sol.lhs
Out[12]: T(t)
In [13]: ode_sol.rhs
Out[13]: C,e-*t + Ta
```

Once the general solution has been found, we need to use the initial conditions to find the values of the yet-to-be-determined integration constants. Here, the initial condition is $T(0) = T_0$. To this end, we first create a dictionary that describes the initial condition, ics = $\{T(0): T0\}$, that we can use with SymPy's subs method to apply the initial condition to the solution of the ODE. This results in an equation for the unknown integration constant C_0 .

```
In [14]: ics = {T(0): T0}
In [15]: ics
Out[15]: {T(0): T<sub>0</sub>}
In [16]: C_eq = ode_sol.subs(t, 0).subs(ics)
In [17]: C_eq
Out[17]: T<sub>0</sub> = C<sub>1</sub> + Ta
```

In the present example, the equation for C_1 is trivial, but for generality, let's solve it using sympy.solve. The result is a list of solutions (in this case a list of only one solution). We can substitute the solution for C_1 into the general solution of the ODE problem to obtain the solution that corresponds to the given initial conditions.

```
In [18]: C_sol = sympy.solve(C_eq)

In [19]: C_sol

Out[19]: [\{C_1: T_0 - T_a\}]

In [20]: ode_sol.subs(C_sol[0])

Out[20]: T(t) = T_a + (T_0 - T_a)e^{-kt}
```

These steps solved the ODE problem symbolically and obtained the solution $T(t) = T_a + (T_0 - T_a)e^{-kt}$. The steps involved in this process are straightforward, but applying the initial conditions and solving for the undetermined integration constants can be slightly tedious, and it is worthwhile to collect these steps in a reusable function. The following function apply_ics is a basic implementation that generalizes these steps to a differential equation of arbitrary order.

```
the form ics = {y(0): y0, y(x).diff(x).subs(x, 0): yp0, ...},
to the solution of the ODE with independent variable x.

The undetermined integration constants C1, C2, ... are extracted
from the free symbols of the ODE solution, excluding symbols in
the known_params list.

"""

free_params = sol.free_symbols - set(known_params)
eqs = [(sol.lhs - sol.rhs).diff(x, n).subs(x, 0).subs(ics)
for n in range(len(ics))]

sol_params = sympy.solve(eqs, free_params)
return sol.subs(sol params)
```

With this function, we can more conveniently single out a particular solution to an ODE that satisfies a set of initial conditions, given the general solution to the same ODE. For the previous example, we get the following.

```
In [22]: ode_sol

Out[22]: T(t) = C_1 e^{-kt} + T_a

In [23]: apply_ics(ode_sol, ics, t, [k, Ta])

Out[23]: T(t) = T_a + (T_o - T_a)e^{-kt}
```

The example we have looked at is almost trivial, but the same method can be used to approach any ODE problem, although there is no guarantee that a solution will be found. As an example of a slightly more complicated problem, consider the ODE for a damped harmonic oscillator, which is a second-order ODE

on the form
$$\frac{d^2x(t)}{dt^2} + 2\gamma\omega_0\frac{dx(t)}{dt} + \omega_0^2x(t) = 0$$
 where $x(t)$ is the position of the oscillator at time t , ω_0 is the

frequency for the undamped case, and γ is the damping ratio. We first define the required symbols, construct the ODE, and then ask SymPy to find the general solution by calling sympy.dsolve.

Since this is a second-order ODE, the general solution has two undetermined integration constants.

We need to specify initial conditions for the position x(0) and the velocity $\frac{dx(t)}{dt}\Big|_{t=0}$ to single out a particular solution to the ODE. To do this, create a dictionary with these initial conditions and apply it to the general ODE solution using apply_ics.

```
In [30]: ics = {x(0): 1, x(t).diff(t).subs(t, 0): 0}
In [31]: ics
```

$$\begin{aligned} & \text{Out[31]: } \left\{ x(0) \!:\! 1, \! \frac{dx(t)}{dt} \right|_{t=0} \!:\! 0 \right\} \\ & \text{In [32]: } x_t_sol = \text{apply_ics(ode_sol, ics, t, [omega0, gamma])} \\ & \text{In [33]: } x_t_sol \\ & \text{Out[33]: } x(t) \!=\! \left(-\frac{\gamma}{2\sqrt{\gamma^2-1}} \!+\! \frac{1}{2} \right) \! e^{\omega_0 t \left(\! -\gamma \! -\sqrt{\gamma^2-1} \right)} \! +\! \left(\frac{\gamma}{2\sqrt{\gamma^2-1}} \! +\! \frac{1}{2} \right) \! e^{\omega_0 t \left(\! -\gamma \! +\sqrt{\gamma^2-1} \right)} \\ \end{aligned}$$

This is the solution for the oscillator dynamics for arbitrary values of t, ω_0 , and γ , where I used the initial condition x(0)=1 and $\frac{dx(t)}{dt}\Big|_{t=0}=0$. However, substituting $\gamma=1$, which corresponds to critical damping,

directly into this expression results in a division by zero error. For this particular choice of γ , we must be careful and compute the limit where $\gamma \rightarrow 1$.

```
In [34]: x_t_critical = sympy.limit(x_t_sol.rhs, gamma, 1) In [35]: x_t_critical  \text{Out}[35]: \frac{\omega_0 t + 1}{e^{\omega_0 t}}
```

Finally, plot the solutions for $\omega_0 = 2\pi$ and a sequence of different values of the damping ratio γ .

```
In [36]: fig, ax = plt.subplots(figsize=(8, 4))
    ...: tt = np.linspace(0, 3, 250)
    \dots: w0 = 2 * sympy.pi
    ...: for g in [0.1, 0.5, 1, 2.0, 5.0]:
             if g == 1:
    . . . :
                  x t expr = x t critical.subs({omega0: w0})
    . . . :
             else:
                 x t expr = x t sol.rhs.subs({omega0: w0, gamma: g})
    . . . :
             x_t = sympy.lambdify(t, x_t_expr, 'numpy')
             ax.plot(tt, x t(tt).real, label=r"$\gamma = %.1f$" % g)
    ...: ax.set_xlabel(r"$t$", fontsize=18)
    ...: ax.set ylabel(r"$x(t)$", fontsize=18)
    ...: ax.legend()
```

The solution to the ODE for the damped harmonic oscillator is graphed in Figure 9-1. For $\gamma < 1$, the oscillator is underdamped, and we see oscillatory solutions. For $\gamma > 1$, the oscillator is overdamped and decays monotonically. The crossover between these two behaviors occurs at the critical damping ratio $\gamma = 1$.

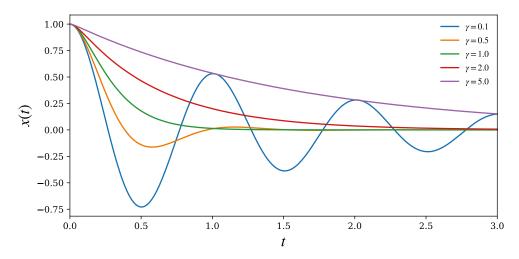


Figure 9-1. Solutions to the ODE for a damped harmonic oscillator for a sequence of damping ratios

The two examples of ODEs we have looked at so far could both be solved exactly by analytical means, but this is far from always the case. Even many first-order ODEs cannot be solved exactly in terms of elementary functions. For example, consider $\frac{dy(x)}{dx} = x + y(x)^2$, which is an example of an ODE that does not have any closed-form solution. If we try to solve this equation using sympy.dsolve, we obtain an approximate solution in the form of a power series (using the hint keyword argument with value '1st_

```
In [37]: x = \text{sympy.symbols}("x")

In [38]: y = \text{sympy.Function}("y")

In [39]: f = y(x)**2 + x

In [40]: \frac{dy(x)}{dx} = x + y(x)^2

In [41]: \text{sympy.dsolve}(y(x).\text{diff}(x) - f, \text{hint='1st_power_series'})

y(x) = C_1 + C_1 x + \frac{1}{2}(2C_1 + 1)x^2 + \frac{7C_1}{6}x^3 + \frac{C_1}{12}(C_1 + 5)x^4
Out[41]: + \frac{1}{60}(C_1^2(C_1 + 45) + 20C_1 + 3)x^5 + \mathcal{O}(x^6)
```

power series').

For many other types of equations, SymPy outright fails to produce any solution at all. For example, if

we attempt to solve the second-order ODE $\frac{d^2y(x)}{dx^2} = x + y(x)^2$, we obtain the following error message.

In [42]: sympy.Eq(y(x).diff(x, x), f)

Out[42]:
$$\frac{d^2y(x)}{dx^2} = x + y(x)^2$$
In [43]: sympy.dsolve(y(x).diff(x, x) - f)
...

NotImplementedError: solve: Cannot solve -x - y(x)**2 + Derivative(y(x), x, x)

This type of result can mean that there is no analytical solution to the ODE or, just as likely, simply that SymPy cannot handle it.

The dsolve function accepts many optional arguments, and it can frequently make a difference if the solver is guided by giving hints about which methods should be used to solve the ODE problem at hand. See the docstring for sympy.dsolve for more information about the available options.

Direction Fields

A *direction field graph* is a simple but useful technique to visualize possible solutions to arbitrary first-order ODEs. It is made up of short lines that show the slope of the unknown function on a grid in the x-y plane. This graph can be easily produced because the slope of y(x) at arbitrary points of the x-y plane is given by

the definition of the ODE: $\frac{dy(x)}{dx} = f(x,y(x))$. That is, we only need to iterate over the x and y values on the

coordinate grid of interest and evaluate f(x, y(x)) to know the slope of y(x) at that point. The direction field graph is useful because smooth and continuous curves that tangent the slope lines (at every point) in the direction field graph are possible solutions to the ODE.

The following function plot_direction_field produces a direction field graph for a first-order ODE, given the independent variable x, the unknown function y(x), and the right-hand side f(x, y(x)) function. It also takes optional ranges for the x and y axes (x_lim and y_lim, respectively) and an optional Matplotlib axis instance to draw the graph on.

```
In [44]: def plot direction field(
                  x, y_x, f_xy, x_lim=(-5, 5), y_lim=(-5, 5), ax=None):
   . . . :
             f_np = sympy.lambdify((x, y_x), f_xy, 'numpy')
   ...:
             x \text{ vec} = \text{np.linspace}(x \text{ lim}[0], x \text{ lim}[1], 20)
   . . . :
             y vec = np.linspace(y lim[0], y lim[1], 20)
   . . . :
             if ax is None:
                  , ax = plt.subplots(figsize=(4, 4))
             dx = x \text{ vec}[1] - x \text{ vec}[0]
             dy = y \ vec[1] - y \ vec[0]
   . . . :
   . . . :
             for m, xx in enumerate(x vec):
                  for n, yy in enumerate(y vec):
                      Dy = f np(xx, yy) * dx
                      Dx = 0.8 * dx**2 / np.sqrt(dx**2 + Dy**2)
                      Dy = 0.8 * Dy*dy / np.sqrt(dx**2 + Dy**2)
                      ax.plot([xx - Dx/2, xx + Dx/2],
                               [yy - Dy/2, yy + Dy/2], 'b', lw=0.5)
             ax.axis('tight')
             ax.set title(r"$%s$" %
   . . . :
                            (sympy.latex(sympy.Eq(y(x).diff(x), f xy))),
                            fontsize=18)
   . . . :
             return ax
   . . . :
```

With this function, we can produce the direction field graphs for the ODEs on the form

 $\frac{dy(x)}{dx} = f(x,y(x))$. For example, the following code generates the direction field graphs for $f(x,y(x)) = y(x)^2 + x$, f(x,y(x)) = -x/y(x), and $f(x,y(x)) = y(x)^2/x$. The result is shown in Figure 9-2.

```
In [45]: x = sympy.symbols("x")
In [46]: y = sympy.Function("y")
In [47]: fig, axes = plt.subplots(1, 3, figsize=(12, 4))
    ...: plot_direction_field(x, y(x), y(x)**2 + x, ax=axes[0])
    ...: plot_direction_field(x, y(x), -x / y(x), ax=axes[1])
    ...: plot_direction_field(x, y(x), y(x)**2 / x, ax=axes[2])
```

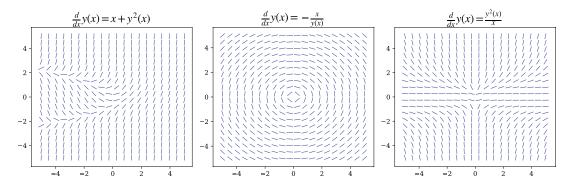


Figure 9-2. Direction fields for three first-order differential equations

The direction lines in the graphs in Figure 9-2 suggest how the curves that are solutions to the corresponding ODE behave, and direction field graphs are a valuable tool for visualizing solutions to ODEs

that cannot be solved analytically. To illustrate this point, consider again the ODE $\frac{dy(x)}{dx} = x + y(x)^2$ with

the initial condition y(0) = 0, which we previously saw can be solved inexactly as an approximate power series. Like before, we solve this problem again by defining the symbol x and the y(x) function, which we, in turn, use to construct and display the ODE.

```
In [48]: x = sympy.symbols("x")

In [49]: y = sympy.Function("y")

In [50]: f = y(x)**2 + x

In [51]: sympy.Eq(y(x).diff(x), f)

Out[51]: \frac{dy(x)}{dx} = x + y(x)^2
```

We want to find the specific power-series solution that satisfies the initial condition. For this problem, we can specify the initial condition directly using the ics keyword argument to the dsolve function.

```
In [52]: ics = {y(0): 0}

In [53]: ode_sol = sympy.dsolve(y(x).diff(x)-f, ics=ics, hint='1st_power_series')

In [54]: ode_sol

Out[54]: y(x) = \frac{x^2}{2} + \frac{x^5}{20} + \mathcal{O}(x^6)
```

Plotting the solution together with the direction field for the ODE is a quick and straightforward way to get an idea of the validity range of the power-series approximation. The following code plots the approximate solution and the direction field (see Figure 9-3, left panel). A solution with an extended validity range is also obtained by repeatedly solving the ODE with initial conditions at increasing values of *x*, taken from a previous power-series solution (see Figure 9-3, right panel).

```
In [55]: fig, axes = plt.subplots(1, 2, figsize=(8, 4))
    ...: # left panel
    ...: plot_direction_field(x, y(x), f, ax=axes[0])
    ...: x \text{ vec} = \text{np.linspace}(-3, 3, 100)
    ...: axes[0].plot(x vec,
                        sympy.lambdify(x, ode_sol.rhs.remove0()) (x_vec), 'b', lw=2)
    ...: axes[0].set ylim(-5, 5)
    . . . :
    ...: # right panel
    ...: plot direction field(x, y(x), f, ax=axes[1])
    ...: x_vec = np.linspace(-1, 1, 100)
    ...: axes[1].plot(x vec,
                        sympy.lambdify(x, ode sol.rhs.remove0()) (x vec), 'b', lw=2)
    ...:
    ...: # iteratively resolve the ODE with updated initial conditions
    ...: ode sol m = ode sol p = ode sol
    ...: dx = 0.125
    ...: # positive x
    ...: for x0 in np.arange(1, 2., dx):
              x \text{ vec} = \text{np.linspace}(x0, x0 + dx, 100)
    ...:
              ics = \{y(x0): ode sol p.rhs.remove0().subs(x, x0)\}
    . . . :
              ode_sol_p = sympy.dsolve(
                  y(x).diff(x) - f, ics=ics, n=6, hint='1st power series')
    ...:
                  x_vec, sympy.lambdify(x, ode_sol_p.rhs.remove0())(x vec),
    . . . :
                  'r', lw=2)
    . . . :
    ...: # negative x
    ...: for x0 in np.arange(-1, -5, -dx):
    . . . :
              x \text{ vec} = \text{np.linspace}(x0, x0 - dx, 100)
```

¹In the current version of SymPy, the ics keyword argument is only recognized by the power-series solver in dsolve. Solvers for other types of ODEs ignore the ics argument; hence the need for the apply_ics function defined and used earlier in this chapter. To guide dsolve to use a power series method, we can use the hint='1st_power_series' argument.

In the left panel of Figure 9-3, the approximate solution curve aligns well with the direction field lines near x = 0 but starts to deviate for $|x| \gtrsim 1$, suggesting that the approximate solution is no longer valid. The solution curve in the right panel aligns better with the direction field throughout the plotted range. The blue (dark gray) curve segment is the original approximate solution, and the red (light gray) curves are continuations obtained from resolving the ODE with an initial condition sequence that starts where the blue (dark gray) curves end.

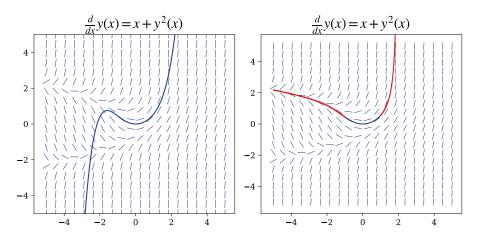


Figure 9-3. Direction field graph of the ODE with the $\frac{dy(x)}{dx} = y(x)^2 + x$ fifth-order power-series solutions around x = 0 (left), and consecutive power-series expansions around x between -5 and x = 0, with a 0.125 spacing (right)

Solving ODEs Using Laplace Transformations

An alternative to solving ODEs symbolically with SymPy's "black-box" solver² dsolve is to use the symbolic capabilities of SymPy to assist in a more manual approach to solving ODEs. A technique that can be used to solve certain ODE problems is to Laplace transform the ODE, which for many problems results in an algebraic equation that is easier to solve. The solution to the algebraic equation can then be transformed back to the original domain with an inverse Laplace transform to obtain the solution to the original problem. The key to this method is that the Laplace transform of the derivative of a function is an algebraic expression in the Laplace transform of the function itself: L[y'(t)] = sL[y(t)] - y(0). However, while SymPy is

 $^{^2}$ Or "white-box" solver, since SymPy is open source and the inner workings of dsolve are readily available for inspection.

good at Laplace transforming many types of elementary functions, it does not recognize how to transform derivatives of an unknown function. But defining a function that performs this task easily amends this shortcoming.

For example, consider the following differential equation for a driven harmonic oscillator.

$$\frac{d^2}{dt^2}y(t) + 2\frac{d}{dt}y(t) + 10y(t) = 2\sin 3t$$

To work with this ODE, first create SymPy symbols for the independent variable t and the y(t) function and then use them to construct the symbolic expression for the ODE.

```
In [56]: t = sympy.symbols("t", positive=True)
In [57]: y = sympy.Function("y")
In [58]: ode = y(t).diff(t, 2) + 2 * y(t).diff(t) + 10 * y(t) - 2 * sympy.sin(3*t)
In [59]: sympy.Eq(ode)
Out[59]: 10y(t)-2\sin(3t)+2\frac{d}{dt}y(t)+\frac{d^2}{dt^2}y(t)=0
```

Laplace transforming this ODE should yield an algebraic equation. To pursue this approach using SymPy and its function sympy.laplace_transform, we first need to create a symbol s, to be used in the Laplace transformation. At this point, we also create a symbol Y for later use.

Next, let's proceed to Laplace transform the unknown function y(t), as well as the entire ODE equation.

```
In [61]: L_y = sympy.laplace_transform(y(t), t, s) In [62]: L_y Out[62]: \mathcal{L}_t[y(t)](s) In [63]: L_ode = sympy.laplace_transform(ode, t, s, noconds=True) In [64]: sympy.Eq(L_ode) Out[64]: 10\mathcal{L}_t[y(t)](s) + 2\mathcal{L}_t[\frac{d}{dt}y(t)](s) + \mathcal{L}_t[\frac{d^2}{dt^2}y(t)](s) - \frac{6}{s^2+9} = 0
```

When Laplace-transforming the unknown function y(t), we get the undetermined result $L_t[y(t)](s)$, which is to be expected. However, applying sympy.laplace_transform on a derivative of y(t), such as

$$\frac{d}{dt}y(t)$$
 , results in the unevaluated expression, $\mathcal{L}_{t}\left[\frac{d}{dt}y(t)\right](s)$. This form is not the desired result, and we

need to work around this issue to obtain the sought-after algebraic equation. The Laplace transformation of the derivative of an unknown function has a well-known form that involves the Laplace transform of the function itself rather than its derivatives. The following formula is the nth derivative of the y(t) function:

$$\mathcal{L}_{t}\left[\frac{d^{n}}{dt^{n}}y(t)\right](s) = s^{n}\mathcal{L}_{t}\left[y(t)\right](s) - \sum_{m=0}^{n-1} s^{n-m-1}\frac{d^{m}}{dt^{m}}y(t)\bigg|_{t=0}.$$

By iterating through the SymPy expression tree for L_ode and replacing the occurrences of $\mathcal{L}_t \left[\frac{d^n}{dt^n} y(t) \right] (s)$ with expressions of the form given by this formula, we can obtain the algebraic form of the ODE that we seek. The following function takes a Laplace-transformed ODE and performs the substitution of the unevaluated Laplace transforms of the derivatives of y(t).

```
In [65]: def laplace_transform_derivatives(e):
             Evaluate laplace transforms of derivatives of functions
    . . . :
    . . . :
             if isinstance(e, sympy.LaplaceTransform):
                 if isinstance(e.args[0], sympy.Derivative):
                      d, t, s = e.args
                      n = d.args[1][1]
                      return (
                           (s**n) * sympy.LaplaceTransform(d.args[0], t, s) -
                          sum([s**(n-i) * sympy.diff(d.args[0], t, i-1).subs(t, 0))
                          for i in range(1, n+1)]))
             if isinstance(e, (sympy.Add, sympy.Mul)):
                 t = type(e)
                  return t(*[laplace transform derivatives(arg)
                              for arg in e.args])
    . . . :
             return e
    . . . :
```

Applying this function on the Laplace-transformed ODE equation, Lode, yields the following.

In [66]: L_ode_2 = laplace_transform_derivatives(L_ode) In [67]: sympy.Eq(L_ode_2)
$$s^2 \mathcal{L}_t \Big[y(t) \Big](s) + 2s \mathcal{L}_t \Big[y(t) \Big](s) - sy(0)$$
 Out[67]:
$$+10 \mathcal{L}_t \Big[y(t) \Big](s) - 2y(0) - \frac{d}{dt} y(t) \Big|_{t=0} - \frac{6}{s^2 + 9} = 0$$

To simplify the notation, now substitute the expression $L_t[y(t)](s)$ for the symbol Y.

In [68]: L_ode_3 = L_ode_2.subs(L_y, Y)
In [69]: sympy.Eq(L_ode_3)
Out[69]:
$$s^2Y + 2sY - sy(0) + 10Y - 2y(0) - \frac{d}{dt}y(t) - \frac{6}{s^2 + 9} = 0$$

At this point, we need to specify the boundary conditions for the ODE problem. Here, use y(0) = 1 and y'(t) = 0, and after creating a dictionary that contains these boundary conditions, use it to substitute the values into the Laplace-transformed ODE equation.

This is an algebraic equation that can be solved for Y.

In [75]: Y_sol = sympy.solve(L_ode_4, Y)
In [76]: Y_sol
Out[76]:
$$\left[\frac{s^3 + 2s^2 + 9s + 24}{s^4 + 2s^3 + 19s^2 + 18s + 90}\right]$$

The result is a list of solutions, which, in this case, contains only one element. Performing the inverse Laplace transformation on this expression gives the solution to the original problem in the time domain.

In [77]: y_sol = sympy.inverse_laplace_transform(Y_sol[0], s, t) In [78]: sympy.simplify(y_sol) Out[78]:
$$\frac{1}{111e^t} (6(\sin 3t - 6\cos 3t)e^t + 43\sin 3t + 147\cos 3t)$$

This technique of Laplace transforming an ODE, solving the corresponding algebraic equation, and inverse Laplace transforming the result to obtain the solution to the original problem can be applied to solve many significant ODE problems that arise in, for example, electrical engineering and process control applications. Although these problems can be solved by hand with the help of Laplace transformation tables, using SymPy has the potential of significantly simplifying the process.

Numerical Methods for Solving ODEs

While some ODE problems can be solved with analytical methods, as shown in previous examples, it is much more common that ODE problems cannot be solved analytically. In practice, ODE problems are mainly solved with numerical methods. There are many approaches to solving ODEs numerically, and most of them are designed for problems formulated as a system of first-order ODEs on the standard form³

$$\frac{d\mathbf{y}(x)}{dx} = f(x,\mathbf{y}(x))$$
, where $\mathbf{y}(x)$ is a vector of unknown functions of x . SciPy provides functions for solving

this kind of problem, but before exploring how to use those functions, let's briefly review the fundamental concepts and introduce the terminology used for the numerical integration of ODE problems.

The basic idea of many numerical methods for ODEs is captured in the Euler method. This method can, for example, be derived from a Taylor series expansion of y(x) around the point x,

$$y(x+h) = y(x) + \frac{dy(x)}{dx}h + \frac{1}{2}\frac{d^2y(x)}{dx^2}h^2 + \dots,$$

where we consider the case when y(x) is a scalar function for notational simplicity. By dropping terms of second order or higher, we get the approximate equation $y(x+h) \approx y(x) + f(x,y(x))h$, which is accurate to first order in the stepsize h. This equation can be turned into an iteration formula by discretizing the x variables, $x_0, x_1, ..., x_k$ choosing the stepsize $h_k = x_{k+1} - x_k$, and denoting $y_k = y(x_k)$. The resulting iteration formula $y_{k+1} \approx y_k + f(x_k, y_k)h_k$ is known as the *forward Euler method*, and it is said to be an *explicit* form because, given the value of the y_k , we can directly compute y_{k+1} using the formula. The goal of the numerical solution of an initial value problem is to compute y(x) at some points x_n , given the initial condition $y(x_0) = y_0$. Therefore, an

³ Recall that any ODE problem can be written as a system of first-order ODEs on this standard form.

iteration formula like the forward Euler method can be used to compute successive values of y_k , starting from y_0 . There are two types of errors involved in this approach. First, the truncation of the Taylor series gives an error that limits the method's *accuracy*. Second, the approximation of y_k provided by the previous iteration when computing y_{k+1} gives an additional error that may accumulate over successive iterations and affect the method's *stability*.

An alternative form, which can be derived in a similar manner, is the *backward Euler method*, given by the iteration formula $y_{k+1} \approx y_k + f(x_{k+1}, y_{k+1})h_k$. This is an example of a *backward differentiation formula* (BDF), which is *implicit* because y_{k+1} occurs on both sides of the equation. To compute y_{k+1} , we must solve an algebraic equation (e.g., using Newton's method, see Chapter 5). Implicit methods are more complicated to implement than explicit methods, and each iteration requires more computational work. However, the advantage is that implicit methods generally have larger stability regions and better accuracy, which means larger stepsize h_k can be used while still obtaining an accurate and stable solution. Whether explicit or implicit methods are more efficient depends on the problem being solved. Implicit methods are often particularly useful for *stiff* problems, which, loosely speaking, are ODE problems that describe dynamics with multiple disparate timescales (e.g., dynamics that include both fast and slow oscillations).

There are several methods to improve upon the first-order Euler forward and backward methods. One strategy is to keep higher-order terms in the Taylor series expansion of y(x+h), which gives higher-order iteration formulas that can have better accuracy, such as the second-order method

 $y_{k+1} \approx y(x_k) + f(x_{k+1}, y_{k+1})h_k + \frac{1}{2}y_k^{''}(x)h_k^2$. However, such methods require evaluating higher-order derivatives of y(x), which may be a problem if f(x, y(x)) is not known in advance (and not given in symbolic form). Ways around this problem include approximating the higher-order derivatives using finite-difference approximations of the derivatives or sampling the f(x, y(x)) function at intermediary points in the interval $[x_k, x_{k+1}]$. An example of this type of method is the well-known Runge-Kutta method, a single-step method that uses additional evaluations of f(x, y(x)). The most well-known Runge-Kutta method is the fourth-order scheme

$$y_{k+1} = y_k + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$

where

$$k_{1} = f(t_{k}, y_{k})h_{k},$$

$$k_{2} = f\left(t_{k} + \frac{h_{k}}{2}, y_{k} + \frac{k_{1}}{2}\right)h_{k},$$

$$k_{3} = f\left(t_{k} + \frac{h_{k}}{2}, y_{k} + \frac{k_{2}}{2}\right)h_{k},$$

$$k_{4} = f(t_{k} + h_{k}, y_{k} + k_{3})h_{k}.$$

Here, k_1 to k_4 are four different evaluations of the ODE f(x, y(x)) function used in the explicit formula for y_{k+1} . The resulting estimate of y_{k+1} is accurate to the fourth order, with an error of the fifth order. Higher-order schemes that use more function evaluations can also be constructed. By combining two methods of different orders, it can be possible also to estimate the error in the approximation. A popular combination is the Runge-Kutta fourth- and fifth-order schemes, which results in a fourth-order accurate method with error estimates. It is known as RK45 or the Runge-Kutta-Fehlberg method. The Dormand-Prince method is another example of a higher-order method that uses adaptive step-size control. For example, the 8-5-3

method combines third- and fifth-order schemes to produce an eighth-order method. An implementation of this method is available in SciPy, which we will see in the next section.

An alternative method is to use more than one previous value of y_k to compute y_{k+1} . Such methods are known as multistep methods and can, in general, be written in the following form.

$$y_{k+s} = \sum_{n=0}^{s-1} a_n y_{k+n} + h \sum_{n=0}^{s} b_n f(x_{k+n}, y_{k+n})$$

With this formula, to compute y_{k+s} , the previous s values of y_k and $f(x_k, y_k)$ are used (known as an s-step method). The choices of the coefficients a_n and b_n give rise to different multistep methods. Note that if $b_s = 0$, the method is explicit; if $b_s \neq 0$, it is implicit.

For example, $b_0 = b_1 = \dots = b_{s-1} = 0$ gives the general formula for an s-step BDF formula, where a_n and b_n are chosen to maximize the order of the accuracy by requiring that the method is exact for polynomials up to as high order as possible. This gives an equation system that can be solved for the unknown coefficients a_n and b_n . For example, the one-step BDF method with $b_1 = a_0 = 1$ reduces to the backward Euler method, $y_{k+1} = y_k + hf(x_{k+1}, y_{k+1})$, and the two-step BDF method, $y_{k+2} = a_0 y_k + a_1 y_{k+1} + hb_2 f(x_{k+2}, y_{k+2})$, when solved for the coefficients $(a_0, a_1, a_1, a_1, b_2)$, becomes $y_{k+2} = -\frac{1}{3}y_k + \frac{4}{3}y_{k+1} + \frac{2}{3}hf(x_{k+2}, y_{k+2})$. Higher-order BDF methods can also be constructed. SciPy provides a BDF solver recommended for stiff problems because of its good

stability properties. Another family of multistep methods is the Adams methods, which result from the choice $a_0 = a_1 = \ldots = a_{s-2} = 0$ and $a_{s-1} = 1$, where again the remaining unknown coefficients are chosen to maximize the order of the method. Specifically, the explicit methods with $b_s = 0$ are known as Adams-Bashforth methods, and the implicit methods with $b_s \neq 0$ are known as Adams-Moulton methods. For example, the

one-step Adams-Bashforth and Adams-Moulton methods reduce to the forward and backward Euler methods, respectively, and the two-step methods are $y_{k+2} = y_{k+1} + h\left(-\frac{1}{2}f\left(x_{k},y_{k}\right) + \frac{3}{2}f\left(x_{k+1},y_{k+1}\right)\right)$ and $y_{k+1} = y_{k} + \frac{1}{2}h\left(f\left(x_{k},y_{k}\right) + f\left(x_{k+1},y_{k+1}\right)\right)$, respectively. Higher-order explicit and implicit methods can also be

constructed in this way. Solvers using these Adams methods are also available in SciPy.

In general, explicit methods are more convenient to implement and less computationally demanding to iterate than implicit methods, which in principle requires solving (a potentially nonlinear) equation in each iteration with an initial guess for the unknown y_{k+1} . However, as mentioned, implicit methods often are more accurate and have superior stability properties. A compromise that retains some of the advantages of both methods is to combine explicit and implicit methods in the following way: first compute y_{k+1} using an explicit method, and then use this y_{k+1} as an initial guess for solving the equation for y_{k+1} given by an implicit method. This equation does not need to be solved exactly, and since the initial guess from the explicit method should be quite good, it could be sufficient with a small number of iterations, using, for example, Newton's method. Methods like these, where the result from an explicit method is used to predict y_{k+1} and an implicit method is used to *correct* the prediction, are called *predictorcorrector* methods.

Finally, an important technique that many advanced ODE solvers employ is *adaptive stepsize* or *stepsize control*: the accuracy and stability of an ODE are strongly related to the stepsize h_k used in the iteration formula for an ODE method, and so is the computational cost of the solution. If the error in y_{k+1} can be estimated together with the computation of y_{k+1} itself, then it is possible to automatically adjust the stepsize h_k so that the solver uses large economical stepsizes when possible and smaller stepsizes when required. A related technique, which is possible with some methods, automatically adjusts the order of the method so that a lower-order method is used when possible and a higher-order method is used when necessary. The Adams methods are examples of methods where the order can be changed easily.

A vast variety of high-quality implementations of ODE solvers exist, and rarely should it be necessary to reimplement any of the methods discussed here. Doing so would probably be a mistake unless it is for educational purposes or if one's primary interest is researching methods for numerical ODE solving.

For practical purposes, it is advisable to use one of the many highly tuned and thoroughly tested ODE suites that already exist, most of which are free and open source and packaged into libraries such as SciPy. However, there are a large number of solvers to choose from, and to be able to make an informed decision on which one to use for a particular problem and to understand many of their options, it is important to be familiar with the basic ideas and methods and the terminology that is used to discuss them.

Numerical Integration of ODEs Using SciPy

After reviewing numerical methods for solving ODEs in the previous section, we are ready to explore the ODE solvers available in SciPy and how to use them. The integrate module of SciPy provides two ODE solver interfaces: integrate.odeint and integrate.ode. The odeint function is an interface to the LSODA solver from ODEPACK, which automatically switches between an Adams predictor-corrector method for nonstiff problems and a BDF method for stiff problems. In contrast, the integrate.ode class provides an object-oriented interface to several different solvers: the VODE and ZVODE solvers (ZVODE is a variant of VODE for complex-valued functions), the LSODA solver, and dopri5 and dop853, which are fourth- and eighth-order Dormand-Prince methods (i.e., types of Runge-Kutta methods) with adaptive stepsize. While the object-oriented interface provided by integrate.ode is more flexible, the odeint function is, in many cases, simpler and more convenient. Let's look at both interfaces, starting with the odeint function.

The odeint function takes three mandatory arguments: a function for evaluating the right-hand side of the ODE on the standard form, an array (or scalar) that specifies the initial condition for the unknown functions, and an array with values of the independent variable where an unknown function is to be computed. The function for the right-hand side of the ODE takes two mandatory arguments and an arbitrary number of optional arguments. The required arguments are the array (or scalar) for the vector y(x) as the first argument and the value of x as the second argument. For example, consider again the scalar ODE $y'(x) = f(x, y(x)) = x + y(x)^2$. To be able to plot the direction field for this ODE again, this time together with a specific solution obtained by numerical integration using odeint, we first define the SymPy symbols required to construct a symbolic expression for f(x, y(x)).

```
In [79]: x = sympy.symbols("x")
In [80]: y = sympy.Function("y")
In [81]: f = y(x)**2 + x
```

To be able to solve this ODE with SciPy's odeint, we first and foremost need to define a Python function for f(x, y(x)) that takes Python scalars or NumPy arrays as input. From the SymPy expression f, we can generate such a function using sympy.lambdify with the 'numpy' argument.⁶

```
In [82]: f np = sympy.lambdify((y(x), x), f, 'numpy')
```

Next, we need to define the initial value y0 and a NumPy array with the discrete values of x for which to compute the y(x) function. Let's solve the ODE starting at x=0 in both the positive and negative directions, using the NumPy arrays xp and xm, respectively. We only need to create a NumPy array with negative increments to solve the ODE in the negative direction. Once we have set up the ODE f_np function, initial value y0, and array of x coordinates, for example, xp, we can integrate the ODE problem by calling integrate.odeint(f_np, y0, xp).

⁴More information about ODEPACK is available at http://computing.llnl.gov/projects/odepack.

⁵The VODE and ZVODE solvers are available at www.netlib.org/ode.

⁶ In this particular case, with a scalar ODE, we could also use the 'math' argument, which produces a scalar function using functions from the standard math library, but more often, array-aware functions are needed. They are obtained by using the 'numpy' argument to sympy.lambdify.

```
In [83]: y0 = 0
In [84]: xp = np.linspace(0, 1.9, 100)
In [85]: yp = integrate.odeint(f_np, y0, xp)
In [86]: xm = np.linspace(0, -5, 100)
In [87]: ym = integrate.odeint(f np, y0, xm)
```

The results are two one-dimensional NumPy arrays ym and yp, of the same length as the corresponding coordinate arrays xm and xp (i.e., 100), which contain the solution to the ODE problem at the specified points. To visualize the solution, plot the ym and yp arrays together with the direction field for the ODE. The result is shown in Figure 9-4. As expected, the solution aligns with (tangents) the lines in the direction field at every point in the graph.

```
In [88]: fig, ax = plt.subplots(1, 1, figsize=(4, 4))
    ...: plot_direction_field(x, y(x), f, ax=ax)
    ...: ax.plot(xm, ym, 'b', lw=2)
    ...: ax.plot(xp, yp, 'r', lw=2)
```

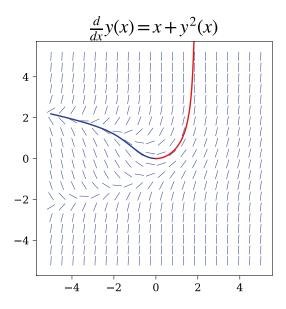


Figure 9-4. The direction field of the ODE $y'(x) = x + y(x)^2$ and the specific solution that satisfies y(0) = 0

The previous example solved a scalar ODE problem. More often, we are interested in vector-valued ODE problems (systems of ODEs). To see how we can solve that kind of problem using odeint, consider the Lotka-Volterra equations for the dynamics of a population of predator and prey animals (a classic example of coupled ODEs). The equations are x'(t) = ax - bxy and y'(t) = cxy - dy, where x(t) is the number of prey animals and y(t) is the number of predator animals, and the coefficients a, b, c, and d describe the rates of the processes in the model. For example, a is the rate at which prey animals are born, and d is the rate at which predators die. The b and c coefficients are the rates at which predators consume prey and the rate at which the predator population grows at the expense of the prey population, respectively. Note that this is a nonlinear system of ODEs because of the xy terms.

To solve this problem with odeint, we first need to write a function for the right-hand side of the ODE in vector form. For this case, we have $f(t, [x, y]^T) = [ax - bxy, cxy - dy]^T$, which we can implement as a Python function in the following way.

This also defined variables and values for the coefficients a, b, c, and d. Note that here, the first argument of the ODE f function is an array containing the current values of x(t) and y(t). For convenience, we first unpack these variables into separate variables, x and y, which makes the rest of the function easier to read. The function's return value should be an array, or list, containing the values of the derivatives of x(t) and y(t). The f function must also take the t argument, with the current value of the independent coordinate. However, t is not used in this example. Once the f function is defined, we must define an array xy0 with the initial values x(0) and y(0) and an array t for the points at which we wish to compute the solution to the ODE. Here, let's use the initial conditions x(0) = 600 and y(0) = 400, corresponding to 600 prey animals and 400 predators at the beginning of the simulation.

```
In [91]: xy0 = [600, 400]
In [92]: t = np.linspace(0, 50, 250)
In [93]: xy_t = integrate.odeint(f, xy0, t)
In [94]: xy_t.shape
Out[94]: (250,2)
```

Calling integrate.odeint(f, xy0, t) integrates the ODE problem and returns an array of shape (250, 2), which contains x(t) and y(t) for each of the 250 values in t. The following code plots the solution as a function of time and in phase space. The result is shown in Figure 9-5.

```
In [95]: fig, axes = plt.subplots(1, 2, figsize=(8, 4))
...: axes[0].plot(t, xy_t[:,0], 'r', label="Prey")
...: axes[0].plot(t, xy_t[:,1], 'b', label="Predator")
...: axes[0].set_xlabel("Time")
...: axes[0].set_ylabel("Number of animals")
...: axes[0].legend()
...: axes[1].plot(xy_t[:,0], xy_t[:,1], 'k')
...: axes[1].set_xlabel("Number of prey")
...: axes[1].set_ylabel("Number of predators")
```

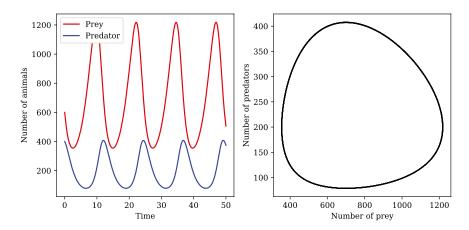


Figure 9-5. A solution to the Lotka-Volterra ODE for predator-prey populations, as a function of time (left) and in phase space (right)

In the previous two examples, the function for the right-hand side of the ODE was implemented without additional arguments. In the example with the Lotka-Volterra equation, the f function used globally defined coefficient variables. Rather than using global variables, it is often convenient and elegant to implement the f function so that it takes arguments for all its coefficients or parameters. To illustrate this point, let's consider another famous ODE problem: the Lorenz equations, which are the following system of three coupled nonlinear ODEs, $x'(t) = \sigma(y-x)$, $y'(t) = x(\rho-z) - y$, and $z'(t) = xy - \beta z$. These equations are known for their chaotic solutions, which sensitively depend on the values of the parameters σ , ρ , and β . Suppose we wish to solve these equations for different values of these parameters. In that case, it is useful to write the ODE function so that it additionally takes the values of these variables as arguments. In the following implementation of f, the three arguments—sigma, rho, and beta—for the corresponding parameters, have been added after the mandatory y(t) and t arguments.

Next, define variables with specific values of the parameters, the array with t values to compute the solution for, and the initial conditions for the x(t), y(t), and z(t) functions.

```
In [97]: sigma, rho, beta = 8, 28, 8/3.0
In [98]: t = np.linspace(0, 25, 10000)
In [99]: xyz0 = [1.0, 1.0, 1.0]
```

This time when we call integrate.odeint, we also need to specify the args argument, which needs to be a list, tuple, or array with the same number of elements as the number of additional arguments in the f function defined in the preceding section. In this case, there are three parameters, and we pass a tuple with the values of these parameters via the args argument when calling integrate.odeint. The following solves the ODE for three different sets of parameters (but the same initial conditions).

```
In [100]: xyz1 = integrate.odeint(f, xyz0, t, args=(sigma, rho, beta))
In [101]: xyz2 = integrate.odeint(f, xyz0, t, args=(sigma, rho, 0.6*beta))
In [102]: xyz3 = integrate.odeint(f, xyz0, t, args=(2*sigma, rho, 0.6*beta))
```

The solutions are stored in the NumPy arrays xyz1, xyz2, and xyz3. In this case, these arrays have the shape (10000, 3) because the t array has 10,000 elements, and there are three unknown functions in the ODE problem. The three solutions are plotted in 3D graphs in the following code, and the result is shown in Figure 9-6. The resulting solutions can vary greatly with small changes in the system parameters.

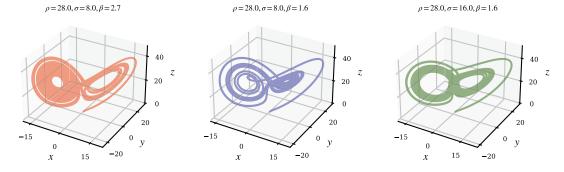


Figure 9-6. The dynamics for the Lorenz ODE for three different sets of parameters

The three examples we have looked at use the odeint solver. This function takes a large number of optional arguments that can be used to fine-tune the solver, including options for the maximum number of allowed steps (hmax) and the maximum order for the Adams (mxordn) and BDF (mxords) methods, to mention a few. See the docstring of odeint for further information.

The alternative to odeint in SciPy is the object-oriented interface provided by the integrate.ode class. Like with the odeint function, to use the integrate.ode class, we first need to define the right-hand side function for the ODE and define the initial state array and an array for the values of the independent variable at which we want to compute the solution. However, one small but important difference is that while the for f(x, y(x)) function to be used with odeint had to have the f(y, x, ...) function signature, the corresponding function to be used with integrate.ode must have the f(x, y, ...) function signature (i.e., the order of x and y is reversed).

The integrate.ode class can work with a collection of different solvers and has specific options for each solver. The docstring of integrate.ode describes the available solvers and their options. To illustrate how to use the integrate.ode interface, let's first look at the following sets of coupled second-order ODEs.

$$m_1 x_1''(t) + \gamma_1 x_1'(t) + k_1 x_1 - k_2 (x_2 - x_1) = 0$$

 $m_2 x_2''(t) + \gamma_2 x_2'(t) + k_2 (x_2 - x_1) = 0$

These equations describe the dynamics of two coupled springs, where
$$\mathbf{x}_1(t)$$
 and $\mathbf{x}_2(t)$ are the displacements of two objects, with masses m_1 and m_2 , from their equilibrium positions. The object at \mathbf{x}_1 is connected to a fixed wall via a spring with spring constant k_1 and connected to the object at \mathbf{x}_2 via a spring with spring constant k_2 . Both objects are subject to damping forces characterized by γ_1 and γ_2 , respectively.

To solve this kind of problem with SciPy, we must first write it in standard form, which we can do by introducing $y_0(t) = x_1(t)$, $y_1(t) = x_1(t)$, $y_2(t) = x_2(t)$, and $y_3(t) = x_2(t)$, which results in four coupled first-order equations.

$$\frac{d}{dt} \begin{bmatrix} y_0(t) \\ y_1(t) \\ y_2(t) \\ y_3(t) \end{bmatrix} = f(t,y(t)) = \begin{bmatrix} y_1(t) \\ (-\gamma_1 y_1(t) - k_1 y_0(t) - k_2 y_0(t) + k_2 y_2(t)) / m_1 \\ y_3(t) \\ (-\gamma_2 y_3(t) - k_2 y_2(t) + k_2 y_0(t)) / m_2 \end{bmatrix}$$

The first task is to write a Python function that implements the f(t, y(t)) function, which also takes the problem parameters as additional arguments. The following implementation bunches all the parameters into a tuple that is passed to the function as a single argument and unpack on the first line of the function body.

The return value of the f function is a list of length 4, whose elements are the derivatives of the ODE $y_0(t)$ to $y_3(t)$ functions. Next, let's create variables with specific values for the parameters and pack them into a tuple args that can be passed to the f function. Like before, we also need to create arrays for the initial condition y0 and for the t values we want to compute the solution to the ODE, t.

```
In [106]: m1, k1, g1 = 1.0, 10.0, 0.5
In [107]: m2, k2, g2 = 2.0, 40.0, 0.25
In [108]: args = (m1, k1, g1, m2, k2, g2)
In [109]: y0 = [1.0, 0, 0.5, 0]
In [110]: t = np.linspace(0, 20, 1000)
```

The main difference between using integrate.odeint and integrate.ode starts at this point. Instead of calling the odeint function, we need to create an instance of the integrate.ode class, passing the ODE f function as an argument.

```
In [111]: r = integrate.ode(f)
```

Here, we store the resulting solver instance in the variable r. Before we can use it, we must configure some of its properties. At a minimum, we need to set the initial state using the set_initial_value method, and if the f function takes additional arguments, we need to configure those using the set_f_params method. We can also select a solver using the set_integrator method, which accepts the following solver names as the first argument: vode, zvode, lsoda, dopri5, and dop853. Each solver takes additional optional arguments. See the docstring for integrate.ode for details. Here, let's use the LSODA solver and set the initial state and the parameters to the f function.

```
In [112]: r.set_integrator('lsoda')
In [113]: r.set_initial_value(y0, t[0])
In [114]: r.set f params(args)
```

Once the solver is created and configured, we can start solving the ODE step by step by calling the r.integrate method, and the status of the integration can be queried using the r.successful method (which returns True as long as the integration is proceeding fine). We need to keep track of which point to integrate to, and we need to store results by ourselves.

```
In [115]: dt = t[1] - t[0]
    ...: y = np.zeros((len(t), len(y0)))
    ...: idx = 0
    ...: while r.successful() and r.t < t[-1]:
    ...: y[idx, :] = r.y
    ...: r.integrate(r.t + dt)
    ...: idx += 1</pre>
```

This is not as convenient as simply calling the odeint, but it offers extra flexibility that sometimes is needed. This example stored the solution in the array y for each corresponding element in t, similar to what odeint would have returned. The following code plots the solution; the result is shown in Figure 9-7.

```
In [116]: fig = plt.figure(figsize=(10, 4))
     ...: ax1 = plt.subplot2grid((2, 5), (0, 0), colspan=3)
     ...: ax2 = plt.subplot2grid((2, 5), (1, 0), colspan=3)
     \dots: ax3 = plt.subplot2grid((2, 5), (0, 3), colspan=2, rowspan=2)
     ...: # x 1 vs time plot
     ...: ax1.plot(t, y[:, 0], 'r')
     ...: ax1.set ylabel('$x 1$', fontsize=18)
     ...: ax1.set_yticks([-1, -.5, 0, .5, 1])
     ...: # x2 vs time plot
     ...: ax2.plot(t, y[:, 2], 'b')
     ...: ax2.set_xlabel('$t$', fontsize=18)
     ...: ax2.set ylabel('$x 2$', fontsize=18)
     ...: ax2.set_yticks([-1, -.5, 0, .5, 1])
     ...: # x1 and x2 phase space plot
     ...: ax3.plot(y[:, 0], y[:, 2], 'k')
     ...: ax3.set_xlabel('$x_1$', fontsize=18)
     ...: ax3.set_ylabel('$x_2$', fontsize=18)
     ...: ax3.set xticks([-1, -.5, 0, .5, 1])
     ...: ax3.set yticks([-1, -.5, 0, .5, 1])
     ...: fig.tight_layout()
```

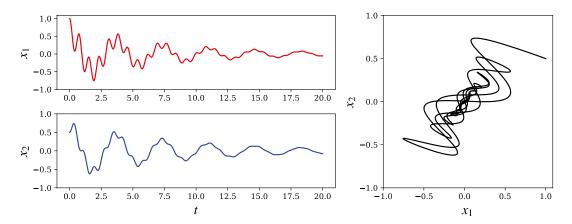


Figure 9-7. The solution of the ODE for two coupled damped oscillators

In addition to providing a Python function for the ODE f(t,y(t)) function, we can also provide a Python function that computes the Jacobian matrix for a given t and y(t). The solver can, for example, use the Jacobian to solve the system of equations that arise in implicit methods more efficiently. To use a Jacobian function jac, like the one defined for the current problem, we must pass it to the integrate.ode class when it is created, together with the f function. If the Jacobian function jac takes additional arguments, those also must be configured using the set_jac_params method in the resulting integrate.ode instance.

Python functions for f(t,y(t)) and its Jacobian can conveniently be generated using SymPy's lambdify, provided that the ODE problem first can be defined as a SymPy expression. This symbolic-numeric hybrid approach is a powerful method for solving ODE problems. To illustrate this approach, consider the rather complicated system of two coupled second-order and nonlinear ODEs for a double pendulum. The equations of motion for the angular deflection, $\theta_1(t)$ and $\theta_2(t)$, for the first and the second pendulum, respectively, are⁷

$$(m_1 + m_2) l_1 \theta_1''(t) + m_2 l_2 \theta_2''(t) \cos(\theta_1 - \theta_2) + m_2 l_2 (\theta_2'(t))^2 \sin(\theta_1 - \theta_2) + g(m_1 + m_2) \sin\theta_1 = 0,$$

$$m_2 l_2 \theta_2''(t) + m_2 l_1 \theta_1'' \cos(\theta_1 - \theta_2) - m_2 l_1 (\theta_1'(t))^2 \sin(\theta_1 - \theta_2) + m_2 g \sin\theta_2 = 0.$$

⁷See http://scienceworld.wolfram.com/physics/DoublePendulum.html for details.

The first pendulum is attached to a fixed support, and the second pendulum is attached to the first. Here m_1 and m_2 are the masses and l_1 and l_2 are the lengths of the first and second pendulums, respectively. Let's begin by defining SymPy symbols for the variables and the functions in the problem and then constructing the ode expressions.

```
In [120]: t, g, m1, l1, m2, l2 = sympy.symbols("t, g, m_1, l_1, m_2, l_2")
In [121]: theta1, theta2 = sympy.symbols("theta 1, theta 2", cls=sympy.Function)
In [122]: ode1 = sympy.Eq(
                  (m1+m2)*l1 * theta1(t).diff(t,t) +
                  m2*l2* theta2(t).diff(t,t)* sympy.cos(theta1(t)-theta2(t)) +
                  m2*l2 * theta2(t).diff(t)**2 * sympy.sin(theta1(t)-theta2(t)) +
                  g*(m1+m2) * sympy.sin(theta1(t)), 0)
      ...: ode1
             g(m_1 + m_2)\sin\theta_1(t) + l_1(m_1 + m_2)\frac{d^2}{dt^2}\theta_1(t) + l_2m_2\sin(\theta_1(t) - \theta_2(t))\left(\frac{d}{dt}\theta_2(t)\right)^2
Out[122]:
             +l_2m_2\frac{d^2}{dt^2}\theta_2(t)\cos(\theta_1(t)-\theta_2(t))=0
In [123]: ode2 = sympy.Eq(
                 m2*l2 * theta2(t).diff(t,t) +
                  m2*l1 * theta1(t).diff(t,t) * sympy.cos(theta1(t)-theta2(t))-
                  m2*l1 * theta1(t).diff(t)**2 * sympy.sin(
                       theta1(t) - theta2(t)) + m2*g * sympy.sin(theta2(t)), 0)
      ...: ode2
             gm_2\sin\theta_2(t)-l_1m_2\sin(\theta_1(t)-\theta_2(t))\left(\frac{d}{dt}\theta_1(t)\right)^2
Out[123]:
             +l_1 m_2 \cos(\theta_1(t) - \theta_2(t)) \frac{d^2}{dt^2} \theta_1(t) + l_2 m_2 \frac{d^2}{dt^2} \theta_2(t) = 0
```

Now, ode1 and ode2 are SymPy expressions for the two second-order ODE equations. Trying to solve these equations with sympy. dsolve is fruitless, and we need to use a numerical method to proceed. However, the equations as they stand here are not in a form that is suitable for numerical solution with the ODE solvers that are available in SciPy. First, we must write the system of two second-order ODEs as a system of four first-order ODEs on the standard form. Rewriting the equations in the standard form is not difficult but can be tedious to do by hand. Fortunately, we can leverage the symbolic capabilities of SymPy to automate this task. To this end, we need to introduce new functions— $y_1(t) = \theta_1(t)$, $y_2(t) = \theta_1'(t)$, $y_3(t) = \theta_2(t)$, and $y_4(t) = \theta_2'(t)$ —and rewrite the ODEs in terms of these functions. By creating a dictionary for the variable change and using the SymPy function subs to perform the substitution using this dictionary, we can easily obtain the equations for $y_2'(t)$ and $y_4'(t)$.

We also need to introduce two more ODEs for $y_1(t)$ and $y_3(t)$.

```
In [128]: ode3 = sympy.Eq(y1(t).diff(t), y2(t))
In [129]: ode4 = sympy.Eq(y3(t).diff(t), y4(t))
```

At this point, we have four coupled first-order ODEs for the y_1 to y_4 functions. It only remains to solve for the derivatives of these functions to obtain the ODEs in standard form. We can do this using sympy.solve.

```
In [130]: y = sympy.Matrix([y1(t), y2(t), y3(t), y4(t)])
In [131]: vcsol = sympy.solve((ode1_vc, ode2_vc, ode3, ode4), y.diff(t), dict=True)
In [132]: f = y.diff(t).subs(vcsol[0])
```

Now, f is the SymPy expression for the ODE f(t,y(t)) function. We can display the ODEs using sympy. Eq(y.diff(t), f), but the result is rather lengthy, and in the interest of space, we do not show the output here. The main purpose of constructing f here is to convert it to a NumPy-aware function that can be used with integrate.odeint or integrate.ode. The ODEs are now on a form that we can create such a function using sympy.lambdify. Also, since there is a symbolic representation of the problem so far, it is easy to compute the Jacobian and create a NumPy-aware function. When using sympy.lambdify to create functions for odeint and ode, we must be careful to put t and y in the correct order in the tuple passed to sympy.lambdify. Here, let's use integrate.ode, so we need a function with the signature f(t, y, *args), and thus we pass the tuple (t, y) as the first argument to sympy.lambdify. We wrap the resulting function with a lambda function to receive the additional argument args, which is not used in the SymPy expression.

```
In [133]: params = {m1: 5.0, l1: 2.0, m2: 1.0, l2: 1.0, g: 10.0}
In [134]: _f_np = sympy.lambdify((t, y), f.subs(params), 'numpy')
In [135]: f_np = lambda _t, _y, *args: _f_np(_t, _y)
In [136]: jac = sympy.Matrix([[fj.diff(yi) for yi in y] for fj in f])
In [137]: _jac_np = sympy.lambdify((t, y), jac.subs(params), 'numpy')
In [138]: jac_np = lambda _t, _y, *args: _jac_np(_t, _y)
```

Here, I have also substituted specific values of the system parameters before calling sympy.lambdify. The first pendulum is twice as long and five times as heavy as the second pendulum. With the f_np and jac_np functions, we are now ready to solve the ODE using integrate.ode in the same manner as in the previous examples. Here, let's take the initial state to be $\theta_1(0) = 2$ and $\theta_2(0) = 0$, and with the derivatives set to zero, solve for the time interval [0, 20] with 1000 steps.

The solution to the ODEs is now stored in the array yy, which has the shape (1000, 4). When visualizing this solution, it is more intuitive to plot the positions of the pendulums in the x – y plane rather than their angular deflections. The transformations between the angular variables θ_1 and θ_2 and x and y coordinates are $x_1 = l_1 \sin \theta_1$, $y_1 = l_1 \cos \theta_1$, $x_2 = x_1 + l_2 \sin \theta_2$, and $y_2 = y_1 + l_2 \cos \theta_2$.

Finally, let's plot the dynamics of the double pendulum as a function of time and in the *x*-*y* plane. The result is shown in Figure 9-8. As expected, pendulum 1 is confined to moving on a circle (because of its fixed anchor point), while pendulum 2 has a much more complicated trajectory.

```
In [145]: fig = plt.figure(figsize=(10, 4))
     ...: ax1 = plt.subplot2grid((2, 5), (0, 0), colspan=3)
     \dots: ax2 = plt.subplot2grid((2, 5), (1, 0), colspan=3)
     \dots: ax3 = plt.subplot2grid((2, 5), (0, 3), colspan=2, rowspan=2)
     ...: ax1.plot(tt, x1, 'r')
     ...: ax1.plot(tt, y1, 'b')
     ...: ax1.set_ylabel('$x_1, y_1$', fontsize=18)
     ...: ax1.set_yticks([-3, 0, 3])
     ...: ax2.plot(tt, x2, 'r')
     ...: ax2.plot(tt, y2, 'b')
     ...: ax2.set_xlabel('$t$', fontsize=18)
     ...: ax2.set ylabel('$x 2, y 2$', fontsize=18)
     ...: ax2.set_yticks([-3, 0, 3])
     ...: ax3.plot(x1, y1, 'r')
     ...: ax3.plot(x2, y2, 'b', lw=0.5)
     ...: ax3.set_xlabel('$x$', fontsize=18)
     ...: ax3.set_ylabel('$y$', fontsize=18)
     ...: ax3.set_xticks([-3, 0, 3])
     ...: ax3.set yticks([-3, 0, 3])
     3
                                                                                 trajectory of pendulum 1
                                                                                 trajectory of pendulum 2
 x_1, y_1
        0.0
                    5.0
                          7.5
                               10.0
                                     12.5
                                            15.0
                                                  17.5
                                                        20.0
     3
 x_2, y_2
        0.0
                    5.0
                                10.0
                                      12.5
                                            15.0
                                                  17.5
                                                        20.0
                                                                    -3
                                                                                   0
                                 t
                                                                                   \boldsymbol{x}
```

Figure 9-8. The dynamics of the double pendulum

Summary

This chapter explored various methods and tools for solving ordinary differential equations (ODEs) using the scientific computing packages for Python. ODEs show up in many areas of science and engineering particularly modeling and the description of dynamical systems—and mastering the techniques to solve ODE problems is a crucial part of the skill set of a computational scientist. The chapter first looked at solving ODEs symbolically using SymPy, either with the sympy.dsolve function or using a Laplace transformation method. The symbolic approach is often a good starting point, and with the symbolic capabilities of SymPy, many fundamental ODE problems can be solved analytically. However, for most practical problems, there is no analytical solution, and the symbolic methods are then doomed to fail. Our remaining option is then to fall back on numerical techniques. Numerical integration of ODEs is a vast field in mathematics, and numerous reliable methods exist for solving ODE problems. The chapter briefly reviewed methods for integrating ODEs, intending to introduce the concepts and ideas behind the Adams and BDF multistep methods used in the solvers provided by SciPy. Finally, we looked at how the odeint and ode solvers, available through the SciPy integrate module, can solve a few example problems. Although most ODE problems eventually require numerical integration, there can be significant advantages in using a hybrid symbolic-numerical approach, which uses features from both SymPy and SciPy. The last example of this chapter is devoted to demonstrating this approach.

Further Reading

An accessible introduction to many methods for numerically solving ODE problems is given in *Scientific Computing* by M. T. Heath (McGraw-Hill, 2002). For a review of ordinary differential equations with code examples, see Chapter 11 in *Numerical Recipes* by W. H. Press et al. (Cambridge University Press, 2007). For a more detailed survey of numerical methods for ODEs, see, for example, (Kendall Atkinson (2009). The main implementations of ODE solvers used in SciPy are the VODE and LSODA solvers. The source code for these methods is available from Netlib at www.netlib.org/odepack, respectively. In addition to these solvers, there is also a well-known suite of solvers called sundials, which the Lawrence Livermore National Laboratory provides and is available at http://computing.llnl.gov/projects/sundials. This suite also includes solvers of differential algebraic equations (DAEs). A Python interface for the sundials solvers is provided by the scikit.odes library, which can be obtained from http://github.com/bmcage/odes. The odespy library also offers a unified interface for many different ODE solvers. For more information about odespy, see the project's website at http://hplgit.github.io/odespy/doc/web/index.html.